10/521,075 Page 1

=> d que 11 1 SEA FILE=CAPLUS ABB=ON PLU=ON WO2001045703/PN L1

=> d bib abs

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
AN
    2001:472491 CAPLUS
DN
    135:76524
TI
    Preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors
    Bandarage, Ramani R.; Bandarage, Upul K.; Fang, Xinqin; Garvey, David S.;
     Letts, L. Gordon; Schroeder, Joseph D.; Tam, Sang William
PA
    Nitromed, Inc., USA
    PCT Int. Appl., 230 pp.
SO
     CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                         KIND
                               DATE
                                           APPLICATION NO.
                                                                   DATE
                               20010628
PΙ
    WO 2001045703
                         A1
                                           WO 2000-US35014
                                                                   20001222
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CR, CU, CZ, DE, DK, DM, D2, EE, ES, FI, GB, GD, GE, GH, GM, HR,
            HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
            YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    CA 2393724
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                                           CA 2000-2393724
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    US 2001041726
                               20011115
                                           US 2000-741816
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    US 6649629
                               20031118
                         B2
                               20021009
    EP 1246621
                         Al
                                           EP 2000-989422
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                                                   20001222
    BR 2000017037
                               20030610
                                           BR 2000-17037
    JP 2003523958
                         T2
                               20030812
                                           JP 2001-546642
                                                                  20001222
                                           NZ 2000-519781
    N2 519781
                               20040430
                                                                  20001222
    AU 782971
                               20050915
                                           AU 2001-25928
                                                                  20001222
                         B2
                                                                   20020717
    ZA 2002005707
                               20031111
                                           ZA 2002-5707
    US 2003220228
                         Al
                               20031127
                                           US 2003-463671
                                                                   20030618
PRAI US 1999-171623P
                         P
                               19991223
    US 2000-226085P
                         P
                               20000818
    US 2000-741816
                               20001222
                         A3
                               20001222
    WO 2000-US35014
    MARPAT 135:76524
GI
```

- L1 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
- AB Title compds. were prepared Thus, MeCOCH: CH2 was condensed with 4-(MeS)C6H4CHO and the oxidized product cyclocondensed with Me2C(SH)CH2NH2
- to give, after Me3CONO treatment, title compound I. Data for biol. activity
- of title compds. were given.
- RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/521,075 Page 3

=> sel l1 1 rn
E1 THROUGH E99 ASSIGNED

=> fil capl
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FILE COVERS 1907 - 15 Aug 2006 VOL 145 ISS 8 FILE LAST UPDATED: 14 Aug 2006 (20060814/ED)

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'.FIONA' IS DEFAULT FORMAT FOR 'CAPLUS' FILE

=> fil reg FILE 'REGISTRY' ENTERED AT 13:30:27 ON 15 AUG 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 14 AUG 2006 HIGHEST RN 901253-54-1 DICTIONARY FILE UPDATES: 14 AUG 2006 HIGHEST RN 901253-54-1

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> => d que l2 stat L2 99 SEA FILE=REGISTRY ABB:

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170571-19-4/BI OR 170571-20-7/BI OR 170571-71-8/BI OR 1778-09-2 /BI OR 179174-91-5/BI OR 179174-92-6/BI OR 179174-93-7/BI OR 179174-94-8/BI OR 18162-48-6/BI OR 181695-72-7/BI OR 181695-81-8/BI OR 189501-33-5/BI OR 189501-34-6/BI OR 194596-99-1/BI OR 205579-90-4/BI OR 205580-05-8/BI OR 213763-90-7/BI OR 213764-17 -1/BI OR 21382-98-9/BI OR 215124-07-5/BI OR 215124-20-2/BI OR 2417-72-3/BI OR 24214-73-1/BI OR 28399-82-8/BI OR 291518-72-4/B I OR 32047-53-3/BI OR 329900-75-6/BI OR 3446-89-7/BI OR 346683-69-0/BI OR 346683-70-3/BI OR 346683-71-4/BI OR 346683-72 -5/BI OR 346683-73-6/BI OR 346683-75-8/BI OR 346683-76-9/BI OR 346683-77-0/BI OR 346683-78-1/BI OR 346683-79-2/BI OR 346683-80 -5/BI OR 346683-81-6/BI OR 346683-82-7/BI OR 346683-83-8/BI OR 346683-84-9/BI OR 346683-85-0/BI OR 346683-86-1/BI OR 346683-87 -2/BI OR 346683-88-3/BI OR 346683-89-4/BI OR 346683-90-7/BI OR 346683-91-8/BI OR 346683-92-9/BI OR 346683-94-1/BI OR 346683-95 -2/BI OR 346683-96-3/BI OR 346683-97-4/BI OR 346683-98-5/BI OR 346683-99-6/BI OR 346684-00-2/BI OR 346684-01-3/BI OR 346684-02 -4/BI OR 346684-03-5/BI OR 346684-04-6/BI OR 346684-05-7/BI OR 346684-06-8/BI OR 346684-07-9/BI OR 346684-08-0/BI OR 346684-09 -1/BI OR 346684-10-4/BI OR 346684-11-5/BI OR 346684-12-6/BI OR 346684-13-7/BI OR 346684-14-8/BI OR 346684-15-9/BI OR 346684-16 -0/BI OR 346684-17-1/BI OR 346684-18-2/BI OR 346684-19-3/BI OR 346684-20-6/BI OR 346684-21-7/BI OR 346684-22-8/BI OR 346684-23 -9/BI OR 347162-90-7/BI OR 347162-91-8/BI OR 40027-88-1/BI OR 52-67-5/BI OR 53-86-1/BI OR 61040-78-6/BI OR 627-18-9/BI OR 73303-88-5/BI OR 78-83-1/BI OR 78-94-4/BI OR 86864-60-0/BI OR 89031-84-5/BI OR 90878-19-6/BI)

=> d 1-99 ide can

L2 ANSWER 1 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

RN 347162-91-8 REGISTRY

Entered STN: 20 Jul 2001

Imidazo[1,2-a]pyridine-7-methanol, 3-(4-fluorophenyl)-2-(4-

(methylsulfonyl)phenyl) - (9CI) (CA INDEX NAME)

3D CONCORD

MF C21 H17 F N2 O3 S

SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

347162-90-7 REGISTRY Entered STN: 20 Jul 2001

3D CONCORD

MF

C21 H16 F N3 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 2 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

STN Files: CA, CAPLUS, USPATZ, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Imidazo[1,2-a]pyridine-7-methanol, 3-(4-fluorophenyl)-2-(4{methylsulfonyl}phenyl}-, nitrate (ester) (9CI) (CA INDEX NAME)

REFERENCE 1: 135:76524

L2 ANSWER 3 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-23-9 REGISTRY

Entered STN: 18 Jul 2001

Butanedioic acid, [(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-, 1-ethyl 4-[2-[4-{1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]ethyl] ester, (22)- (9CI) (CA INDEX NAME)

STEREOSEARCH MF C28 H31 C1 N2 O9 S2

SR

STN Files: CA, CAPLUS, USPAT2, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 4 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-22-8 REGISTRY

Entered STN: 18 Jul 2001 lH-Pyrazole-1-ethanol, 3-[4-(methylsulfonyl)phenyl]-4-(phenylmethyl)-

(9CI) (CA INDEX NAME) 3D CONCORD

MF C19 H20 N2 O3 S

SR CA STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 5 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-21-7 REGISTRY

Entered STN: 18 Jul 2001

Benzenepropanoic acid, 4-(methylthio)- β -oxo- α -(phenylmethyl)-,

ethyl ester (9CI) (CA INDEX NAME)

3D CONCORD

C19 H20 O3 \$ MF 5R

STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 7 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-19-3 REGISTRY

Entered STN: 18 Jul 2001

D-Valine, 3-[[(2,4,6-trimethoxyphenyl)methyl]thio]- (9CI) (CA INDEX

NAME)

FS STEREOSEARCH

MF C15 H23 N O5 S SR CA

STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:575 REFERENCE 2: 135:288343 REFERENCE 3: 135:76524

L2 ANSWER 6 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-20-6 REGISTRY

Entered STN: 18 Jul 2001 ED

1H-Pyrazole-1-ethanol, 3-[4-(methylthio)phenyl]-4-(phenylmethyl)- (9CI) CN

(CA INDEX NAME) 3D CONCORD

C19 H20 N2 O S MF

SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 8 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-18-2 REGISTRY

Entered STN: 18 Jul 2001 1H-Pyrazole-3-methanol, 1-cyclohexyl-5-[4-(methylsulfonyl)phenyl]- (9CI)

(CA INDEX NAME) OTHER NAMES:

4-[1-Cyclohexyl-3-(hydroxymethyl)pyrazol-5-yl]-1-(methylsulfonyl)benzene

FS 3D CONCORD

C17 H22 N2 O3 S SR CA

STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE) REFERENCE 1: 140:423618

REFERENCE 2: 140:77146 REFERENCE 3: 135:76524

ANSWER 9 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN RN 346684-17-1 REGISTRY

Entered STN: 18 Jul 2001

1H-Pyrazole-3-methanol, 1-cyclohexyl-5-[4-(methylthio)phenyl]- (9CI) (CA

[1-Cyclohexyl-5-{4-methylthiophenyl)pyrazol-3-yl]methanol

£2 3D CONCORD

C17 H22 N2 O S MF SR

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:423618 REFERENCE 2: 140:77146 REFERENCE 3: 135:76524

ANSWER 11 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-15-9 REGISTRY

Entered STN: 18 Jul 2001

2-Butenoic acid, 2-hydroxy-4-[4-(methylthio)phenyl]-4-oxo-, methyl ester,

(22) - (9CI) (CA INDEX NAME) OTHER NAMES:

Methyl (2Z)-2-hydroxy-4-(4-methylthiophenyl)-4-oxobut-2-enoate

F5 STEREOSEARCH

MF C12 H12 O4 S SR CA

STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATZ, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE) 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:423618 REFERENCE 2: 140:157441 REFERENCE 3: 140:77147 REFERENCE 4: 140:77146 5: 140:77144 REFERENCE

REFERENCE 6: 135:76524

ANSWER 10 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-16-0 REGISTRY

Entered STN: 18 Jul 2001

1H-Pyrazole-3-carboxylic acid, 1-cyclohexyl-5-[4-(methylthio)phenyl]-, methyl ester (9CI) (CA INDEX NAME)

Methyl 1-cyclohexyl-5-(4-methylthiophenyl)pyrazole-3-carboxylate CN

3D CONCORD F5 MF C18 H22 N2 O2 S

5R

STN Files: CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:423618 REFERENCE 2: 140:77147 REFERENCE 3: 140:77146 REFERENCE 4: 140:77144 REFERENCE 5: 135:76524

ANSWER 12 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-14-8 REGISTRY

Entered STN: 18 Jul 2001

1H-Pyrazole-1-ethanol, 5-[4-(methylsulfonyl)phenyl]-4-(phenylmethyl)-(9CI) (CA INDEX NAME)

3D CONCORD

C19 H20 N2 O3 S

SR CA STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 13 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-13-7 REGISTRY

Entered STN: 18 Jul 2001

1H-Pyrazole-1-ethanol, 5-{4-(methylthio)phenyl]-4-(phenylmethyl)- (9CI)

3D CONCORD

MF C19 H20 N2 O 5

SR STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 15 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-11-5 REGISTRY Entered STN: 18 Jul 2001

Benzoic acid, 4-[[5-(4-fluorophenyl)-4-[4-(methylsulfonyl)phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

3D CONCORD

C26 H21 F N2 O5 S

CA STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 14 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-12-6 REGISTRY

Entered STN: 18 Jul 2001

CN 3(2H)-Pyridazinone, 4-(4-fluorophenyl)-2-[[4-(hydroxymethyl)phenyl]methyl]-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

3D CONCORD

MF C25 H21 F N2 O4 S

LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 16 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-10-4 REGISTRY

Entered STN: 18 Jul 2001

Butanamide, 3-mercapto-3-methyl-N-[[4-(5-methyl-3-phenyl-4-isoxazolyl)phenyl]sulfonyl}- (9CI) (CA INDEX NAME)

3D CONCORD

C21 H22 N2 O4 S2

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L2 ANSWER 17 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 346684-09-1 REGISTRY
ED Entered STN: 18 Jul 2001
CN Butanamide, 3-methyl-N-[[4-(5-methyl-3-phenyl-4-
isoxazolyl)phenyl]sulfonyl]-3-[((2,4,6-trimethoxyphenyl)methyl]thio)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C31 H34 N2 O7 S2
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
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PAGE 2-A

PAGE 1-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 18 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN RN 346684-08-0 REGISTRY
ED Entered STN: 18 Jul 2001
CN Thionitrous acid (HNOS),
S-[1-[3-(2-hydroxyethyl)-2-oxo-4-oxazolidinyl]-1methylethyl] ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C8 H14 N2 O4 S
SR CA

STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

HO-CH₂-CH₂ S-NO

LC

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:424343
REFERENCE 2: 139:350474
REFERENCE 3: 135:76524

L2 ANSWER 17 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued)
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

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L2 ANSWER 19 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 346684-07-9 REGISTRY
ED Entered STN: 18 Jul 2001
CN 2-Oxazolidinone, 3-(2-hydroxyethyl)-4-(1-mercapto-1-methylethyl)- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C8 H15 N O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

HO-CH2-CH2
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2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REFERENCE 1: 141:424343

ANSWER 20 OF 99 . REGISTRY COPYRIGHT 2006 ACS on STN

346684-06-8 REGISTRY

Entered STN: 18 Jul 2001

2-Oxazolidinone, 3-[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-4-[1-methyl-1-[[(2,4,6-trimethoxyphenyl)methyl]thio]ethyl]- (9CI) (CA INDEX

3D CONCORD

C24 H41 N 06 S Si MF

STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:424343

REFERENCE 2: 135:76524

ANSWER 22 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-04-6 REGISTRY

Entered STN: 18 Jul 2001 Thionitrous acid (HNOS),

S-[1-[3-(3-hydroxypropyl)-2-oxo-4-oxazolidinyl]-1-

methylethyl) ester (9CI) (CA INDEX NAME)

3D CONCORD FS

C9 H16 N2 O4 S MF SR

STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474 REFERENCE 2: 135:76524

ANSWER 21 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-05-7 REGISTRY

ED Entered STN: 18 Jul 2001

Benzeneacetamide, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-4-fluoro-N-(2-mercapto-2-methylpropyl)-

N-methyl-, (a2)- (9CI) (CA INDEX NAME) STEREOSEARCH

C24 H28 F N O5 S2 ME

SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 23 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-03-5 REGISTRY Entered STN: 18 Jul 2001 2-Oxazolidinone, 3-(3-hydroxypropyl)-4-(1-mercapto-1-methylethyl)- (9CI) (CA INDEX NAME) 3D CONCORD FS MF C9 H17 N O3 S

(CH2)3-OH

SR CA

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

LC 5TN Files: CA, CAPLUS, USPATZ, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 24 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-02-4 REGISTRY

ED Entered STN: 18 Jul 2001

2-Oxazolidinone,

3-{3-[((1,1-dimethylethyl)dimethylsilyl]oxy]propyl]-4-[1methyl-1-[[(2,4,6-trimethoxyphenyl)methyl]thio]ethyl]- (9CI) (CA INDEX NAME)

3D CONCORD

MF C25 H43 N 06 S Si

STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 26 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346684-00-2 REGISTRY

Entered STN: 18 Jul 2001

1-Butanol, 2-amino-3-methyl-3-[[(2,4,6-trimethoxyphenyl)methyl]thio]-

(9CI) (CA INDEX NAME)

3D CONCORD

MF C15 H25 N O4 S

SR CA STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

L2 ANSWER 25 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346684-01-3 REGISTRY

Entered STN: 18 Jul 2001

2-Oxazolidinone, 4-[1-methyl-1-[{(2,4,6-trimethoxyphenyl)methyl]thio]ethyl

]- (9CI) (CA INDEX NAME) 3D CONCORD FS

C16 H23 N O5 S MF

SR CA STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:424343 REFERENCE 2: 135:76524

ANSWER 27 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 346683-99-6 REGISTRY

Entered STN: 18 Jul 2001

2-Butene-1, 4-dio1, 2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl)-,

1-acetate, (22)- (9CI) (CA INDEX NAME)

STEREOSEARCH

MF C19 H19 F O5 S SR

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 28 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-98-5 REGISTRY

Entered STN: 18 Jul 2001

1H-Pyrrole-1-ethanethiol, a,a,2-trimethyl-5-[4-(methylsulfonyl)phenyl)- (9CI) (CA INDEX NAME)

3D CONCORD

C16 H21 N 02 S2 MF

SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 30 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

RN 346683-96-3 REGISTRY

Entered STN: 18 Jul 2001 Butanamide, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-N-(2-mercapto-2-methylpropyl)-, (22) - (9CI) (CA INDEX NAME)

STEREOSEARCH C28 H40 Cl N O4 S2 Si

MF SR

STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 29 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-97-4 REGISTRY

Entered STN: 18 Jul 2001

Butanamide, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4hydroxy-N-(2-mercapto-2-methylpropyl)-, (2Z)- (9CI) (CA INDEX NAME)

STEREOSEARCH

MF C22 H26 C1 N O4 52 SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

346683-95-2 REGISTRY RN Entered STN: 18 Jul 2001 Butanoic acid, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4-

ANSWER 31 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

hydroxy-, (2Z)- (9CI) (CA INDEX NAME)

STEREOSEARCH C18 H17 C1 O5 S

MF CI COM

SR

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 32 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-94-1 REGISTRY

Entered STN: 18 Jul 2001

1H-Indole-3-acetamide,

1-{4-chlorobenzoyl}-N-(2-mercapto-2-methylpropyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

3D CONCORD

C23 H25 C1 N2 O3 S SR CA

STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 34 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-91-8 REGISTRY

Entered STN: 18 Jul 2001 Thionitrous acid (HNOS), S-[4-(2-hydroxyethyl)-1-methyl-4-piperidinyl)

ester (9CI) (CA INDEX NAME)

3D CONCORD MF C8 H16 N2 O2 S

SR STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474

REFERENCE 2: 135:288343

REFERENCE 3: 135:76524

ANSWER 33 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-92-9 REGISTRY

Entered STN: 18 Jul 2001

1H-Indole, 3-{2-bromoethyl}-1-[(4-chlorophenyl)methyl}-5-methoxy-2-methyl-

(9CI) (CA INDEX NAME) 3D CONCORD

C19 H19 Br C1 N O MF

> CA STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 35 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-90-7 REGISTRY

Entered STN: 18 Jul 2001 4-Piperidineethanol, 1-methyl-4-[(phenylmethyl)thio]- (9CI) (CA INDEX

NAME)

MF C15 H23 N O S

SR CA STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:288343

L2 ANSWER 36 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-89-4 REGISTRY

Entered STN: 18 Jul 2001

4-Piperidineacetic acid, 1-methyl-4-[(phenylmethyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)

3D CONCORD

MF C17 H25 N 02 S

CI COM SR

STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:288343 REFERENCE 2: 135:76524

02N-0-CH2

346683-88-3 REGISTRY

3D CONCORD

C17 H21 N3 O5 S

MF

\$R

Entered STN: 18 Jul 2001

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

nitrate (ester) (9CI) (CA INDEX NAME)

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 37 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

1H-Pyrazole-3-methanol, 1-cyclohexyl-5-[4-(methylsulfonyl)phenyl}-,

STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATZ, USPATFULL

REFERENCE 1: 140:423618 REFERENCE . 2: 135:76524

ANSWER 38 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN L2 346683-87-2 REGISTRY Entered STN: 18 Jul 2001 1H-Pyrazole-1-ethanol, 5-[4-(methylsulfonyl)phenyl)-4-(phenylmethyl)-,

nitrate (ester) (9CI) (CA INDEX NAME)

3D CONCORD

MF C19 H19 N3 O5 S

LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

02N-0-CH2-CH2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 39 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-86-1 REGISTRY Entered STN: 18 Jul 2001

3(2H)-Pyridazinone,

4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-2-[[4-[(nitrooxy)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

3D CONCORD FS

MF C25 H20 F N3 O6 S

SR CA

STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 40 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-85-0 REGISTRY

Entered STN: 18 Jul 2001

1H-Pyrazole-3-carboxylic acid, 1-[4-(aminosulfonyl)phenyl}-5-(4chlorophenyl)-, 2-methyl-2-(nitrosothio)propyl ester (9CI) (CA INDEX NAME)

3D CONCORD FS

C20 H19 C1 N4 O5 S2 MF

SR STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474 REFERENCE 2: 135:76524

ANSWER 42 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-83-8 REGISTRY

Entered STN: 18 Jul 2001

Benzenezcetic acid, α -{2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene}-4-fluoro-,

2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester, (αZ) - (9CI) (CA INDEX NAME)

STEREOSEARCH

C27 H31 F N2 O7 S2 MF SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

ANSWER 41 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

346683-84-9 REGISTRY

Entered STN: 18 Jul 2001

Thionitrous acid (HNOS), $S-\{1,1-dimethyl-3-[[\{4-(5-methyl-3-phenyl-4-(5-methyl-3-($ isoxazolyl)phenyl}sulfonyl]amino]-3-oxopropyl} ester (9CI) (CA INDEX NAME)

3D CONCORD

MF C21 H21 N3 O5 S2 SR

STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

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ANSWER 43 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    346683-82-7 REGISTRY
    Entered STN: 18 Jul 2001
    Thionitrous acid (HNOS),
S-[2-[[(2Z)-4-(acetyloxy)-2-(4-fluorophenyl)-3-[4-
     (methylsulfonyl)phenyl]-1-oxo-2-butenyl]methylamino]-1,1-dimethylethyl)
    ester (9CI) (CA INDEX NAME)
    STEREOSEARCH
MF
    C24 H27 F N2 O6 S2
SR
    STN Files: CA, CAPLUS, USPAT2, USPATFULL
```

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 44 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

RN 346683-81-6 REGISTRY

D Entered STN: 18 Jul 2001

Benzeneacetic acid, $\alpha-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester, (<math>\alpha$ Z)- {9CI} (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H31 F N2 O9 S2 p

SR CA

LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

L2 ANSWER 46 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

RN 346683-79-2 REGISTRY ED Entered STN: 18 Jul 2001

CN Thionitrous acid (HNOS), S-[2-[[(2Z)-2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4-hydroxy-1-oxobutyl]amino]-1,1-dimethylethyl] ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C22 H25 C1 N2 O5 S2 SR CA

LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

L2 ANSWER 45 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

RN 346683-80-5 REGISTRY

ED Entered STN: 18 Jul 2001

- CN Thionitrous acid (HNOS), S-[1,1-dimethyl-2-[2-methyl-5-[4-(methylsulfonyl)phenyl]-lH-pyrrol-1-yl]ethyl} ester (9CI) (CA INDEX

NAME) FS 3D CONCORD

MF C16 H20 N2 O3 S2

SR CA LC STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474
REFERENCE 2: 135:76524

L2 ANSWER 47 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

RN 346683-78-1 REGISTRY ED Entered STN: 18 Jul 2001

CN Butanoic acid, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4-

(nitrooxy)-, (2Z)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C18 H16 C1 N O7 S

MF C18 H16 C1 N O7 S SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 48 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
- 346683-77-0 REGISTRY
- Entered STN: 18 Jul 2001
- Butanoic acid, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4-CN (nitrooxy)-, ethyl ester, (22)- (9CI) (CA INDEX NAME)
- STEREOSEARCH
- MF C20 H20 C1 N O7 S
- SR STN Files: CA, CAPLUS, USPATZ, USPATFULL

Double bond geometry as shown.

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
 - 1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

- ANSWER 50 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
- 346683-75-8 REGISTRY
- Entered STN: 18 Jul 2001
- 2H-1-Benzopyran-3-carboxylic acid, 6-chloro-8-[(nitrooxy)methyl]-2-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)
- MF C14 H11 C1 F3 N O6 SR CA
- LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
 - 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- REFERENCE 1: 135:76524

- L2 ANSWER 49 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
- 346683-76-9 REGISTRY
- Entered STN: 18 Jul 2001
- Thionitrous acid (HNOS),
- S-[2-[[[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl]acetyl]amino]-1,1-dimethylethyl] ester (9CI) (CA INDEX NAME)
- 3D CONCORD
- C23 H24 C1 N3 O4 S MF CA
- SR STN Files: CA, CAPLUS, USPATZ, USPATFULL

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
 - 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- REFERENCE 1: 135:76524

- L2 ANSWER 51 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 346683-73-6 REGISTRY
- Entered STN: 18 Jul 2001 1H-Indole-3-ethanol, 1-[(4-chlorophenyl)methyl]-5-methoxy-2-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C19 H19 C1 N2 O4
- SR CA LC STN Files: CA, CAPLUS, USPATZ, USPATFULL

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
 - 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 52 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 346683-72-5 REGISTRY
ED Entered STN: 18 Jul 2001
CN Butanoic acid,
4-{{[4-(5-methyl-3-phenyl-4-isoxazolyl)phenyl]sulfonyl}amin
o]-4-oxo-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester,
2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)
MF C28 H32 N4 O7 S2 . x C6 H8 O7
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

CM 1

CRN 346683-71-4
CMF C28 H32 N4 O7 S2

L2 ANSWER 53 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 346683-71-4 REGISTRY
ED Entered STN: 18 Jul 2001

4-[[{4-(5-methyl-3-phenyl-4-isoxazolyl)phenyl]sulfonyl]amin
o]-4-oxo-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester (9CI)
(CA INDEX NAME)

FS 3D CONCORD
MF C28 H32 N4 O7 S2
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

PAGE 1-A

Butanoic acid,

PAGE 2-A

CH2
CH2
CH2
Me

L2 ANSWER 52 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

CM 2 CRN 77-92-9 CMF C6 H8 O7

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474
REFERENCE 2: 135:76524

L2 ANSWER 53 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued) **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474
REFERENCE 2: 135:76524

2: 135:76524

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 144:266814
REFERENCE 2: 135:76524

329900-75-6 REGISTRY

Entered STN: 04 Apr 2001 Synthetase, prostaglandin endoperoxide, 2 (9CI) (CA INDEX NAME) OTHER NAMES: CN Arachidonate cyclooxygenase 2 COX 2 CN COX-2 COX2 Cyclooxygenase 2 CN CN Cyclooxygenase II Prostaglandin endoperoxidase synthase 2 CN Prostaglandin endoperoxide H synthase-2 CN Prostaglandin endoperoxide synthase-2 CN Prostaglandin endoperoxide synthetase 2 Prostaglandin G/H synthase-2 CN Prostaglandin H synthase-2 MF Unspecified CI MAN 5R CA STN Files: BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER, USPATZ, USPATFULL LC *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT** 8996 REFERENCES IN FILE CA (1907 TO DATE) 9 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 9053 REFERENCES IN FILE CAPLUS (1907 TO DATE) REFERENCE 1: 145:145984

ANSWER 56 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

REFERENCE 2: 145:145748 REFERENCE 3: 145:143866 REFERENCE 4: 145:143864 REFERENCE 5: 145:142896 REFERENCE 6: 145:142631 REFERENCE 7: 145:142464 REFERENCE 8: 145:142463 REFERENCE 9: 145:142461 REFERENCE 10: 145:142423 L2 ANSWER 55 OF 99 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 346683-69-0 REGISTRY
ED Entered STN: 18 Jul 2001
CN Benzenesulfonamide,
4-[5-(4-chlorophenyl)-3-{(nitrooxy)methyl)-1H-pyrazol1-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H13 C1 N4 O5 S
SR CA

STN Files: CA, CAPLUS, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

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L2 ANSWER 57 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 291518-72-4 REGISTRY
ED Entered STN: 28 Sep 2000
CN Thionitrous acid (HNOS), S-(2-hydroxy-1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C4 H9 N O2 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL
S-NO
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350474

REFERENCE 2: 135:76524

REFERENCE 3: 133:350026

REFERENCE 4: 133:222496

Me - C - CH2 - OH

Me

ANSWER 58 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 215124-20-2 REGISTRY

Entered STN: 03 Dec 1998

2H-1-Benzopyran-3-carboxylic acid, 6-chloro-8-(hydroxymethyl)-2-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

SR CA

STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE) 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524 REFERENCE 2: 133:43440 REFERENCE 3: 132:293665 REFERENCE 4: 129:330653

ANSWER 60 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 213764-17-1 REGISTRY Entered STN: 05 Nov 1998 3(2H)-Pyridazinone, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-(9CI) (CA INDEX NAME) 3D CONCORD MF C17 H13 F N2 O3 5 SR STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:318510 REFERENCE 2: 135:76524 REFERENCE 3: 132:321867 REFERENCE 4: 130:223284 REFERENCE 5: 129:275920

L2 ANSWER 59 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

215124-07-5 REGISTRY Entered STN: 03 Dec 1998 ED

2H-1-Benzopyran-3-carboxylic acid,

6-chloro-8-formyl-2-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

C14 H10 C1 F3 O4 MF SR

STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE) 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524 REFERENCE 2: 133:43440 REFERENCE 3: 132:293665 REFERENCE 4: 129:330653

ANSWER 61 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 213763-90-7 REGISTRY Entered STN: 05 Nov 1998

3(2H)-Pyridazinone, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-2-(phenylmethyl) - (9CI) (CA INDEX NAME) 3D CONCORD

MF C24 H19 F N2 O3 S

SR CA STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:318510 REFERENCE 2: 135:76524 REFERENCE 3: 132:321867 REFERENCE 4: 130:223284 REFERENCE 5: 129:275920

L2 ANSWER 62 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 205580-05-8 REGISTRY
ED Entered STN: 17 May 1998
CN Butanedioic acid, [(4-chlorophenyl)][4-(methylsulfonyl)phenyl]methylene}-,
1-ethyl ester, (22)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN Butanedioic acid, [(4-chlorophenyl)][4-(methylsulfonyl)phenyl]methylene}-,
1-ethyl ester, (2)
OTHER NAMES:
CN
(Z)-3-(Ethoxycarbonyl)-4-(4-chlorophenyl)-4-[4-(methanesulfonyl)phenyl]-3butenoic acid
FS STEREOSEARCH
MF C20 H19 C1 O6 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE) 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

REFERENCE 2: 134:131419

REFERENCE 3: 132:222434

REFERENCE 4: 131:299282

REFERENCE 5: 129:245034

REFERENCE 6: 128:270440

STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

LC

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

18 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 144:318603
REFERENCE 2: 141:424343
REFERENCE 3: 140:399698
REFERENCE 4: 139:175861
REFERENCE 5: 137:352471
REFERENCE 6: 137:310693
REFERENCE 7: 137:279361
REFERENCE 8: 136:401912
REFERENCE 9: 136:53915
REFERENCE 10: 136:53755

ANSWER 63 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN 205579-90-4 REGISTRY Entered STN: 17 May 1998 Butanoic acid, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4hydroxy-, ethyl ester, (2Z)- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES: Butanoic acid, 2-[(4-chlorophenyl)[4-(methylsulfonyl)phenyl]methylene]-4hydroxy-, ethyl ester, (2)-OTHER NAMES: (Z)-Ethyl 3-{4-chlorophenyl}-3-[4-(methanesulfonyl)phenyl}-2-(2hydroxyethyl)-2-propenoate STEREOSEARCH C20 H21 C1 O5 S MF SR CA STN Files: CA, CAPLUS, TOXCENTER, USPATZ, USPATFULL Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

REFERENCE 2: 134:131419

REFERENCE 3: 132:222434

REFERENCE 4: 131:299282

REFERENCE 5: 131:199617

REFERENCE 6: 129:245034

REFERENCE 7: 128:270440

L2 ANSWER 65 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 189501-34-6 REGISTRY
ED Entered STN: 06 Jun 1997
CN 1,4-Pentanedione, 1-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-[4-(Methylsulfonyl)phenyl]pentane-1,4-dione
FS 3D CONCORD
MF C12 H14 O4 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:19242
REFERENCE 2: 135:76524
REFERENCE 3: 132:35714
REFERENCE 4: 129:81660
REFERENCE 5: 126:338393

```
L2 ANSWER 66 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 189501-33-5 REGISTRY
ED Entered STN: 06 Jun 1997
CN 1,4-Pentanedione, 1-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H14 O2 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, USPAT2, USPATFULL
```

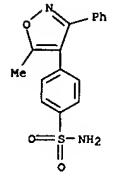
4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:19242
REFERENCE 2: 135:76524
REFERENCE 3: 129:81660
REFERENCE 4: 126:338393

```
181695-72-7 REGISTRY
     Entered STN: 10 Oct 1996
     Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX
     NAME)
OTHER NAMES:
     4-(5-Methyl-3-phenylisoxazol-4-yl)benzenesulfonamide
    Bextra
CN
    SC 65872
ÇN
    Valdecoxib
CN
    Valecoxib
    3D CONCORD
FS
    C16 H14 N2 O3 S
MF
CI
SR
     STN Files: ADISINSIGHT, ANABSTR, BIOSIS, BIOTECHNO, CA, CAPLUS,
       CASREACT, CBNB, CHEMCATS, CSCHEM, EMBASE, HSDB*, IMSDRUGNEWS,
      IMSPATENTS, IMSRESEARCH, IPA, MRCK*, PATDPASPC, PHAR, PROUSDDR, PS,
       RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
```

(*File contains numerically searchable property data)

ANSWER 68 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN



L2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

575 REFERENCES IN FILE CA (1907 TO DATE)
25 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
580 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 145:138598

REFERENCE 2: 145:137889

REFERENCE 3: 145:137255

REFERENCE 4: 145:131074

REFERENCE 5: 145:124547

REFERENCE 6: 145:110313

REFERENCE 7: 145:90062

REFERENCE 8: 145:80979

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

50 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
50 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:460064
REFERENCE 2: 143:378975
REFERENCE 3: 142:170033
REFERENCE 4: 142:168948
REFERENCE 5: 141:134107
REFERENCE 6: 140:368700
REFERENCE 7: 140:229475
REFERENCE 8: 140:192031
REFERENCE 9: 140:175165
REFERENCE 10: 140:138676

L2 ANSWER 68 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued) REFERENCE 9: 145:76198

ANSWER 69 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

179174-94-8 REGISTRY

Entered STN: 07 Aug 1996

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-CN (methylsulfonyl)phenyl]ethylidene]-4-fluoro-, (aZ)- (9CI) (CA INDEX

OTHER CA INDEX NAMES:

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene)-4-fluoro-, (2)-

C19 H17 F O6 S MF

SR CA

STN Files: CA, CAPLUS, USPAT2, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

REFERENCE 2: 125:114294

ANSWER 71 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN RN

179174-92-6 REGISTRY

Entered STN: 07 Aug 1996

2-Butene-1,4-diol, 2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-,4-acetate, (2Z)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

2-Butene-1, 4-diol, 2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl)-, 4-acetate, (Z)-

STEREOSEARCH FS

C19 H19 F 05 S MF

SR

STN Files: CA, CAPLUS, USPAT2, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

REFERENCE 2: 125:114294

ANSWER 70 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

179174-93-7 REGISTRY

Entered STN: 07 Aug 1996

Benzeneacetaldehyde, $\alpha - (2 - (acetyloxy) - 1 - (4 - (acetyloxy) - 1))$ (methylsulfonyl)phenyl]ethylidene]-4-fluoro-, (aZ)- (9CI) (CA INDEX

OTHER CA INDEX NAMES:

Benzeneacetaldehyde, a-[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, (2)-

MF C19 H17 F O5 S

STN Files: CA, CAPLUS, USPAT2, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

REFERENCE 2: 125:114294

```
ANSWER 72 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
179174-91-5 REGISTRY
Entered STN: 07 Aug 1996
```

2-Butene-1,4-diol, 2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-, (22) -

(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES: 2-Butene-1,4-diol, 2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-, (Z)-CN

STEREOSEARCH C17 H17 F O4 S MF

SR STN Files: CA, CAPLUS, USPAT2, USPATFULL LC

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524 REFERENCE 2: 125:114294

```
ANSWER 73 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
```

170571-71-8 REGISTRY

Entered STN: 23 Nov 1995

Benzenesulfonamide, 4-{5-(4-chlorophenyl)-3-(hydroxymethyl)-1H-pyrazol-1yl)- (9CI) (CA INDEX NAME) OTHER NAMES:

4-[5-(4-Chlorophenyl)-3-(hydroxymethyl)pyrazolyl]benzenesulfonamide

FS 3D CONCORD

MF C16 H14 C1 N3 O3 S CA

SR STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

40 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA . 40 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:170033

REFERENCE 2: 141:134107

REFERENCE 3: 140:229475

REFERENCE 4: 140:175165

REFERENCE 5: 140:105282

REFERENCE 6: 140:77146

REFERENCE 7: 140:35975

REFERENCE 8: 140:23256

REFERENCE 9: 140:13075

REFERENCE 10: 139:374217

ANSWER 75 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

170571-19-4 REGISTRY Entered STN: 23 Nov 1995

1H-Pyrazole-3-carboxylic acid, 1-[4-(aminosulfonyl)phenyl]-5-(4-

chlorophenyl) - (9CI) (CA INDEX NAME)

3D CONCORD

MF C16 H12 C1 N3 O4 S

SR STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATZ, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE) 11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14058

REFERENCE 2: 136:369710

REFERENCE 3: 136:69808

REFERENCE 4: 135:76524

REFERENCE 5: 129:54367

REFERENCE 6: 126:317377

REFERENCE 7: 126:264035 REFERENCE 8: 126:104081

REFERENCE 9: 126:104079

REFERENCE 10: 125:114612

ANSWER 74 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

170571-20-7 REGISTRY

Entered STN: 23 Nov 1995 1H-Pyrazole-3-carboxylic acid, 1-[4-(aminosulfonyl)phenyl]-5-(4-

chlorophenyl) -, methyl ester (9CI) (CA INDEX NAME)

3D CONCORD

MF C17 H14 C1 N3 O4 S SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE) 10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14058

2: 136:369710 REFERENCE

REFERÈNCE 3: 136:69808

REFERENCE 4: 135:76524

REFERENCE 5: 129:54367

REFERENCE 6: 126:317377

REFERENCE 7: 126:264035

REFERENCE 8: 126:104081

REFERENCE 9: 126:104079

REFERENCE 10: 123:340112

ANSWER 76 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

157672-00-9 REGISTRY

Entered STN: 15 Sep 1994

2(5H)-Furanone, 3-(4-fluorophenyl)-4-(4-(methylsulfonyl)phenyl)- (9CI) (CA INDEX NAME)

3-(4-fluorophenyl)-4-[4-(methylsulfonyl)phenyl]-5H-furan-2-one

FS MF

C17 H13 F O4 S SR

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19 REFERENCES IN FILE CA (1907 TO DATE) 19 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:316514

REFERENCE 2: 141:420034 REFERENCE 3: 141:16893

REFERENCE 4: 139:78424

REFERENCE 5: 135:76524

REFERENCE 6: 131:193918

REFERENCE 7: 130:24965

REFERENCE 8: 128:13139

REFERENCE 9: 127:247929

REFERENCE 10: 126:301785

```
L2 ANSWER 77 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 136881-95-3 REGISTRY
ED Entered STN: 25 Oct 1991
CN 1H-Indole-3-ethanol, 1-[(4-chloropheny1)methy1)-5-methoxy-2-methyl- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C19 H20 C1 N 02
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
```

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:76524

REFERENCE 2: 128:13200

REFERENCE 3: 115:269798

REFERENCE

REFERENCE

REFERENCE

REFERENCE

REFERENCE

REFERENCE

REFERENCE

REFERENCE

2: 145:83577

3: 145:62923

4: 145:62874

5: 145:46092

6: 145:28135

7: 145:27907

8: 145:24458

9: 145:21189

REFERENCE 10: 144:488445

```
ANSWER 78 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    90878-19-6 REGISTRY
    Entered STN: 16 Nov 1984
ED
    Magnesium, chloro(2-phenylethyl) - (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    Benzene, ethyl-, magnesium complex
OTHER NAMES:
    (2-Phenylethyl) magnesium chloride
    Phenethylmagnesium chloride
    C8 H9 C1 Mg
    STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, GMELIN*,
      TOXCENTER, USPAT2, USPATFULL
        (*File contains numerically searchable property data)
Ph-CH2-CH2-Mg-Cl
            107 REFERENCES IN FILE CA (1907 TO DATE)
            107 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1: 145:83315
REFERENCE
          2: 144:445377
           3: 144:432541
REFERENCE
REFERENCE
          4: 144:370129
REFERENCE
           5: 144:331748
REFERENCE
           6: 144:331055
REFERENCE 7: 144:232928
           8: 144:192094
REFERENCE
REFERENCE 9: 144:51675
REFERENCE 10: 143:477992
```

```
ANSWER 79 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    89031-84-5 REGISTRY
     Entered STN: 16 Nov 1984
    Silane, (3-bromopropoxy) (1,1-dimethylethyl) dimethyl- (9CI) (CA INDEX
    NAME)
OTHER NAMES:
     (3-Bromopropoxy) (1,1-dimethylethyl)dimethylsilane
     (3-Bromopropoxy)-tert-butyldimethylsilane
CN
     1-Bromo-3-{(tert-butyldimethylsilanyl)oxy]propane
CN
    1-Bromo-3-((tert-butyldimethylsilyl)oxy)propane
     3-((tert-Butyldimethylsilyl)oxy)-1-bromopropane
CN
CN
    3-(tert-Butyldimethylsilyloxy)bromopropane
    3-(tert-Butyldimethylsilyloxy)propyl bromide
CN
    3-Bromo-1-(1,1,2,2-tetramethyl-1-silapropoxy)propane
    3-Bromo-1-(tert-butyldimethylsilyloxy)propane
CN
CN
    3-Bromo-1-tert-butyldimethylsiloxypropane
CN
    3-Bromo-1-[(1,1,2,2-tetramethyl-1-silapropyl)oxy]propane
     [(3-Bromopropyl)oxy](1,1-dimethylethyl)dimethylsilane
F5
    3D CONCORD
MF
    C9 H21 Br O Si
    STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX,
       TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
    9- (CH2)3-Br
Me-si-Bu-t
   Me
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             231 REFERENCES IN FILE CA (1907 TO DATE)
              1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             231 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE
           1: 145:103438
```

```
ANSWER 80 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    86864-60-0 REGISTRY
    Entered STN: 16 Nov 1984
    Silane, (2-bromoethoxy) (1,1-dimethylethyl) dimethyl- (9CI) (CA INDEX
NAME)
OTHER NAMES:
     (2-Bromoethoxy) (1,1-dimethylethyl) dimethylsilane
CN
     (2-bromoethoxy) (tert-butyl) dimethylsilane
    1-(tert-Butyldimethylsilyloxy)-2-bromoethane
CN
    1-Bromo-2-[(tert-butyldimethylsilyl)oxy]ethane
CN
    2-(tert-Butyldimethylsilyloxy)-1-bromoethane
CN
CN
    2-(tert-Butyldimethylsilyloxy)bromoethane
    2-(tert-Butyldimethylsilyloxy)ethyl bromide
CN
    2-Bromoethoxy-tert-butyldimethylsilane
     2-Bromoethyl tert-butyldimethylsilyl ether
CN
CN
     2-Bromoethyloxy(tert-butyl)dimethylsilane
CN
     [(2-Bromoethyl)oxy](1,1-dimethylethyl)dimethylsilane
FS
    3D CONCORD
    C8 H19 Br O Si
MF
     STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM,
       SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
    Q-CH2-CH2Br
Me Si Bu-t
   Мe
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             237 REFERENCES IN FILE CA (1907 TO DATE)
             237 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE
           1: 145:124780
REFERENCE
           2: 145:103917
REFERENCE
           3: 145:79107
REFERENCE
           4: 145:46047
REFERENCE
           5: 144:488968
REFERENCE
           6: 144:432827
REFERENCE
           7: 144:432552
REFERENCE
           8: 144:412531
REFERENCE 9: 144:390925
REFERENCE 10: 144:345996
```

```
ANSWER 81 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    73303-88-5 REGISTRY
    Entered STN: 16 Nov 1984
ED
CN
    1-Propanol, 2-mercapto-2-methyl- (7CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
    2-(Hydroxymethyl)propane-2-thiol
    2-Mercapto-2, 2-dimethylethanol
CN
    2-Mercapto-2-methyl-1-propanol
CN
    2-Methyl-2-mercapto-1-propanol
CN
    2-Methyl-2-mercaptopropanol-1
F5
    3D CONCORD
    C4 H10 O 5
MF
    STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPAT2,
      USPATFULL
         (*File contains numerically searchable property data)
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19 REFERENCES IN FILE CA (1907 TO DATE)
19 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 143:326636
REFERENCE 2: 135:76524
REFERENCE 3: 133:350026
REFERENCE 4: 133:222496
REFERENCE 5: 125:115085
REFERENCE 6: 124:146699
REFERENCE 7: 123:9873
REFERENCE 8: 119:203357
REFERENCE 9: 118:124965
REFERENCE 10: 115:233745

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:54158
REFERENCE 2: 135:76524
REFERENCE 3: 84:59566
REFERENCE 4: 78:97599

L2 ANSWER 82 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61040-78-6 REGISTRY
ED Entered 5TN: 16 Nov 1984
CN Benzenemethanol, 2,4,6-trimethoxy- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2,4,6-Trimethoxybenzyl alcohol
FS 3D CONCORD
MF C10 H14 04
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,
USPAT2, USPATFULL

(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

34 REFERENCES IN FILE CA (1907 TO DATE) 35 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 144:318603

REFERENCE 2: 144:274304

REFERENCE 3: 141:424343

REFERENCE 4: 140:399698

REFERENCE 5: 140:390446

REFERENCE 6: 139:350474

REFERENCE 7: 139:175861

REFERENCE 8: 137:352471

REFERENCE 9: 137:310693

REFERENCE 10: 137:279361

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37 REFERENCES IN FILE CA (1907 TO DATE)
37 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 144:274288 REFERENCE 2: 144:232858 REFERENCE 3: 142:141216 REFERENCE 4: 141:424343 REFERENCE 5: 141:174191 REFERENCE 6: 139:350474 REFERENCE 7: 138:369172 REFERENCE 8: 138:214391 REFERENCE 9: 137:310693 REFERENCE 10: 137:279361

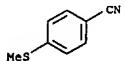
```
ANSWER 85 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    28399-82-8 REGISTRY
    Entered STN: 16 Nov 1984
    Acetic acid, (1-methyl-4-piperidinylidene)-, ethyl ester (9CI) (CA INDEX
    NAME)
OTHER CA INDEX NAMES:
    \Delta 4, \alpha-Piperidineacetic acid, 1-methyl-, ethyl ester (8CI)
OTHER NAMES:
    NSC 121144
CN
    3D CONCORD
FS
    C10 H17 N Q2
MF
CI
    COM
    STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMEN, TOXCENTER,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
```

19 REFERENCES IN FILE CA (1907 TO DATE) 19 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:288343 REFERENCE 2: 135:76524 REFERENCE 3: 134:366772 REFERENCE 4: 130:267275 REFERENCE 5: 126:104080 REFERENCE 6: 124:117151 REFERENCE 7: 124:8763 REFERENCE 8: 124:8585 REFERENCE 9: 120:323116 REFERENCE 10: 120:270063

```
21382-98-9 REGISTRY
     Entered STN: 16 Nov 1984
    Benzonitrile, 4-{methylthio}- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    Benzonitrile, p-(methylthio) - (6CI, 7CI, 8CI)
OTHER NAMES:
    1-Cyano-4-(methylthio) benzene
CN
     4- (Methylthio) benzonitrile
    4-Cyanophenyl methyl sulfide
CN
    4-Methylsulfanylbenzonitrile
CN
    Methyl 4-cyanophenyl sulfide
     Methyl p-cyanophenyl sulfide
CN
     p-(Methylthio)benzonitrile
CN
     p-Cyanophenyl methyl sulfide
FS
     3D CONCORD
MF
    C8 H7 N S
     STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
       CHEMINFORMRX, CSCHEM, SPECINFO, TOXCENTER, USPATFULL
         (*File contains numerically searchable property data)
```

ANSWER 87 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

157 REFERENCES IN FILE CA (1907 TO DATE) 157 REFERENCES IN FILE CAPLUS (1907 TO DATE) 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
REFERENCE 1: 145:145326
REFERENCE
          2: 145:103252
REFERENCE 3: 144:487275
REFERENCE 4: 144:467861
REFERENCE
         5: 144:342565
REFERENCE
           6: 144:291350
REFERENCE
           7: 144:274134
REFERENCE
           8: 144:170752
REFERENCE 9: 143:286353
REFERENCE 10: 143:267006
```

```
ANSWER 86 OF 99 REGISTRY COPYRIGHT 2006 ACS ON STN
    24214-73-1 REGISTRY
    Entered STN: 16 Nov 1984
    Hydrazine, cyclohexyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
    Cyclohexylhydrazine hydrochloride
    Cyclohexylhydrazine monohydrochloride
    C6 H14 N2 . C1 H
STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM,
MF
      TOXCENTER, USPATZ, USPATFULL
         (*File contains numerically searchable property data)
    (6498-34-6)
      . ин- ин2
   HC1
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
              43 REFERENCES IN FILE CA (1907 TO DATE)
             43 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1: 144:450725
REFERENCE
           2: 142:373824
           3: 142:155945
REFERENCE
REFERENCE
          4: 142:74598
           5: 141:395577
REFERENCE
REFERENCE
           6: 141:332110
REFERENCE 7: 141:207202
REFERENCE 8: 140:423618
REFERENCE 9: 140:357383
REFERENCE 10: 140:339323
```

```
L2 ANSWER 88 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    18162-48-6 REGISTRY
     Entered STN: 16 Nov 1984
    Silane, chloro(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Silane, chloro-tert-butyldimethyl- (BCI)
OTHER NAMES:
     (1,1-Dimethylethyl)dimethylsilyl chloride
ÇN
CN
     Chloro(1,1-dimethylethyl)dimethylsilane
     Chloro-tert-butyldimethylsilane
CN
    Chlorodimethyl-tert-butylsilane
     Dimethyl (1, 1-dimethylethyl) chlorosilane
     Dimethyl-tert-butylchlorosilane
CN
     Dimethyl-tert-butylsilyl chloride
CN
     t-Butyldimethylchlorosilane
CN
     TBDMS chloride
    TBDMS-C1
CN
     tert-Butylchlorodimethylsilane
     tert-Butyldimethylchlorosilane
     tert-Butyldimethylsilyl chloride
CN
     3D CONCORD
F$
    132560-73-7, 187979-91-5
DR
    C6 H15 C1 Si
     STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
       CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, GMELIN*, IFICDB,
       IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PROMT, PS, RTECS*, SPECINFO,
       SYNTHLINE, TOXCENTER, USPAT7, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources: EINECS**, NDSL**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
Me Si Bu-t
   Me
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
            4414 REFERENCES IN FILE CA (1907 to DATE)
             39 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
           4423 REFERENCES IN FILE CAPLUS (1907 TO DATE)
              2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
REFERENCE
           1: 145:147869
REFERENCE
           2: 145:145757
REFERENCE 3: 145:145553
REFERENCE
          4: 145:145290
REFERENCE
           5: 145:145275
```

REFERENCE

6: 145:133913

REFERENCE 7: 145:124764

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L2 ANSWER 88 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE 8: 145:124613

REFERENCE 9: 145:124570

REFERENCE 10: 145:124461
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ANSWER 89 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
     15581-80-3 REGISTRY
     Entered STN: 16 Nov 1984
ED
     Propanal, 2,2'-dithiobis(2-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    Propionaldehyde, 2,2'-dithiobis(2-methyl- (7CI, 8CI)
OTHER NAMES:
    \alpha, \alpha'-Dithiobis (isobutyraldehyde)
CN
CN
    a,a'-Dithiodiisobutyraldehyde
    2,2'-Dithiobis(2-methylpropanal)
    2,2'-Dithiobis(2-methylpropionaldehyde)
    2,2'-Dithiobisisobutyraldehyde
     2,2'-Dithiodiisobutyraldehyde
CN
    2,2,5,5-Tetramethyl-3,4-dithiahexanedial
     Diisobutyraldehyde disulfide
     Dithiodiisobutyraldehyde
     3D CONCORD
    C8 H14 O2 S2
MF
CI
     COM
     STN Files: AQUIRE, BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMLIST,
       IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources: DSL**
         (**Enter CHEMLIST File for up-to-date regulatory information)
```

3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
98 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 144:44525

REFERENCE 2: 143:326636

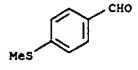
REFERENCE 3: 142:129835

98 REFERENCES IN FILE CA (1907 TO DATE)

REFERENCE 4: 141:424343
REFERENCE 5: 141:97028
REFERENCE 6: 140:52180
REFERENCE 7: 139:85005
REFERENCE 8: 138:149608

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L2 ANSWER 89 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE 9: 137:272430
REFERENCE 10: 137:256878
```

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L2 ANSWER 90 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    3446-89-7 REGISTRY
    Entered STN: 16 Nov 1984
    Benzaldehyde, 4-(methylthio)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzaldehyde, p-(methylthio)- (6CI, 7CI, 8CI)
OTHER NAMES:
    4-{Methylmercapto}benzaldehyde
CN
CN
    4-(Methylthio)benzaldehyde
    4-Methanesulfanylbenzaldehyde
CN
    4-Methanethiobenzaldehyde
CN
     4-Methylsulfanylbenzaldehyde
CN
    Methyl 4-formylphenyl thioether
    p-(Methylthio)benzaldehyde
    3D CONCORD
FS
MF
    C8 H8 O S
CI
    COM
    STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
      CHEMINFORMRX, CHEMLIST, CSCHEM, IFICDB, IFIPAT, IFIUDB, PS, SPECINFO,
      SYNTHLINE, TOXCENTER, USPAT7, USPATFULL
        (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
```



REFERENCE

```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
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1: 145:137267

677 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
680 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 2: 145:123959
REFERENCE 3: 145:123949
REFERENCE 4: 145:103431
REFERENCE 5: 145:103430
REFERENCE 6: 145:57131
REFERENCE 7: 145:46088
REFERENCE 8: 144:488379
REFERENCE 9: 144:488111
REFERENCE 10: 144:467988

(Continued)

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ANSWER 91 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
     2417-72-3 REGISTRY
    Entered STN: 16 Nov 1984
ED
    Benzoic acid, 4-(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    p-Toluic acid, α-bromo-, methyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
    α-Bromo-p-toluic acid methyl ester
    4-{Bromomethyl}benzoic acid methyl ester
    4-{Carbomethoxy}benzyl bromide
    4-(Methoxycarbonyl)benzyl bromide
    Methyl a-bromo-p-toluate
CN
     Methyl 4-(bromomethyl)benzoate
     Methyl p-(bromomethyl)benzoate
CN
     NSC 83959
CN
     p-(Bromomethyl)benzoic acid methyl ester
     p-(Carbomethoxy)benzyl bromide
     p-(Methoxycarbonyl)benzyl bromide
     3D CONCORD
    C9 H9 Br O2
    STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, IFICDB, IFIPAT, IFIUDB, PS, SPECINFO, SYNTHLINE,
       TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             872 REFERENCES IN FILE CA (1907 TO DATE)
              3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             873 REFERENCES IN FILE CAPLUS (1907 TO DATE)
               7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
REFERENCE 1: 145:145348
REFERENCE 2: 145:103688
REFERENCE 3: 145:103565
REFERENCE 4: 145:83296
REFERENCE 5: 145:78748
REFERENCE 6: 145:63132
```

```
ANSWER 92 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    1776-09-2 REGISTRY
    Entered STN: 16 Nov 1984
   Ethanone, 1-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
   Acetophenone, 4'-{methylthio}- (6CI, 7CI, 8CI)
OTHER NAMES:
    1-(4-Methylsulfanylphenyl)ethanone
    1-{4-(Methylthio)phenyl)ethanone
CN
    4'-(Methylmercapto)acetophenone
    4'-(Methylthio)acetophenone
CN
    4-Acetylphenyl methyl sulfide
CN
    4-Acetylthioanisole
    Methyl 4-(methylthio) phenyl ketone
CN
CN
    Methyl p-acetylphenyl sulfide
CN
    NSC 403927
    p-(Methylmercapto) acetophenone
CN
    p-(Methylthio)acetophenone
CN
    p-Acetylphenyl methyl sulfide
CN
    p-Acetylthicanisole
FS
    3D CONCORD
    C9 H10 O S
CI
    COM
LC
    STN Files: AQUIRE, BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
      CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, PS,
       SYNTHLINE, TOXCENTER, USPATZ, USPATFULL
         (*File contains numerically searchable property data)
    Other Sources: EINECS**
         (**Enter CHEMLIST File for up-to-date regulatory information)
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

284 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 286 REFERENCES IN FILE CAPLUS (1907 TO DATE) 14 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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REFERENCE 1: 145:103252
REFERENCE
          2: 145:83244
REFERENCE 3: 145:62680
REFERENCE 4: 145:62670
REFERENCE 5: 144:468011
REFERENCE 6: 144:350708
REFERENCE 7: 144:342565
```

REFERENCE 9: 145:46017 REFERENCE 10: 145:20398

L2 ANSWER 91 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

REFERENCE 7: 145:55355

REFERENCE 8: 145:46221

REFERENCE 10: 144:128531

ANSWER 92 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued) REFERENCE 8: 144:311952 REFERENCE 9: 144:192197

(Continued)

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ANSWER 93 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    1445-73-4 REGISTRY
   Entered STN: 16 Nov 1984
   4-Piperidinone, 1-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4-Piperidone, 1-methyl- (6CI, 7CI, 8CI)
OTHER NAMES:
   1-Methyl-4-oxopiperidine
    1-Methyl-4-piperidinone
CN
    1-Methyl-4-piperidone
CN
    N-Methyl-4-piperidinone
    N-Methyl-4-piperidone
CN
    NSC - 66491
    3D CONCORD
FS
    C6 H11 N O
MF
    COM
    STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
      CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, IFICDB, IFIPAT, IFIUDB, PIRA,
      PS, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
        (*File contains numerically searchable property data)
    Other Sources: EINECS**
        (**Enter CHEMLIST File for up-to-date regulatory information)
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
            884 REFERENCES IN FILE CA (1907 TO DATE)
             4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            887 REFERENCES IN FILE CAPLUS (1907 TO DATE)
             4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
REFERENCE 1: 145:124578
REFERENCE 2: 145:83390
           3: 145:83388
REFERENCE
REFERENCE
           4: 145:83387
REFERENCE
           5: 145:83386
REFERENCE 6: 145:83385
REFERENCE 7: 145:83185
    ANSWER 94 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    627-18-9 REGISTRY
    Entered STN: 16 Nov 1984
    1-Propanol, 3-bromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Bromo-3-hydroxypropane
    1-Bromo-3-propanol
    3-Bromo-1-propanol
    3-Bromopropyl alcohol
CN
    3-Hydroxypropyl bromide
    Trimethylene bromohydrin
CN
FS
    3D CONCORD
    C3 H7 Br O
MF
    COM
CI
    STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
      CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE, GMELIN*, IFICDB, IFIPAT,
IFIUDB,
      PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPATZ, USPATFULL
        (*File contains numerically searchable property data)
    Other Sources: EINECS**, NDSL**, TSCA**
        (**Enter CHEMLIST File for up-to-date regulatory information)
Br-CH2-CH2-CH2-OH
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
           1424 REFERENCES IN FILE CA (1907 TO DATE)
             18 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
           1427 REFERENCES IN FILE CAPLUS (1907 TO DATE)
              B REFERENCES IN FILE CAOLD (PRIOR TO 1967)
REFERENCE 1: 145:130561
REFERENCE 2: 145:126119
REFERENCE 3: 145:124764
REFERENCE 4: 145:103662
REFERENCE 5: 145:103438
REFERENCE 6: 145:103362
REFERENCE 7: 145:83577
REFERENCE 8: 145:83314
REFERENCE 9: 145:83244
REFERENCE 10: 145:62924
```

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L2 ANSWER 95 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
    100-53-8 REGISTRY
    Entered STN: 16 Nov 1984
    Benzenemethanethiol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN
    a-Toluenethiol (7CI, 8CI)
OTHER NAMES:
     (Mercaptomethyl) benzene
CN
    a-Mercaptotoluene
    \alpha-Toluolthiol
CN
CN
    \alpha-Tolyl mercaptan
    Benzyl mercaptan
CN
    Benzylthiol
ÇN
    NSC 41897
CN
     Phenylmethanethiol
CN
     Phenylmethyl mercaptan
CN
    Thiobenzyl alcohol
CN
     3D CONCORD
FS
     C7 H8 S
MF
CI
    COM
    STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS,
       CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, DETHERM*,
       EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MRCK*, MSDS-OHS,
      NAPRALERT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2,
USPATFULL
         (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
HS-CH2-Ph
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
            3650 REFERENCES IN FILE CA (1907 TO DATE)
             66 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            3657 REFERENCES IN FILE CAPLUS (1907 TO DATE)
              5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
REFERENCE 1: 145:154323
REFERENCE 2: 145:145894
REFERENCE 3: 145:145424
REFERENCE
          4: 145:145322
REFERENCE
          5: 145:145070
REFERENCE
           6: 145:144985
REFERENCE
           7: 145:124281
REFERENCE
           8: 145:124231
REFERENCE 9: 145:124133
REFERENCE 10: 145:123941
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L2 ANSWER 93 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

REFERENCE 8: 145:63142

REFERENCE 10: 144:390735

REFERENCE 9: 145:290

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Page 31
                                                                                      L2 ANSWER 96 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
L2 ANSWER 95 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
                                                           (Continued)
                                                                                           78-94-4 REGISTRY
                                                                                          Entered STN: 16 Nov 1984
                                                                                           3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)
                                                                                      OTHER NAMES:
                                                                                           1-Buten-3-one
                                                                                      CN
                                                                                           2-Butenone
                                                                                      CN
                                                                                           3-0xo-1-butene
                                                                                           3-Oxobutene
                                                                                           Methyl vinyl ketone
                                                                                           NSC 4853
                                                                                           Vinyl methyl ketone
                                                                                      CN
                                                                                           3D CONCORD
                                                                                      FS
                                                                                           C4 H6 O
                                                                                      MF
                                                                                      CI
                                                                                           COM
                                                                                           STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO,
                                                                                             CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST,
                                                                                             CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPLIT, ENCOMPLIT2,
                                                                                             ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE,
                                                                                             MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SPECINFO,
                                                                                             SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL
                                                                                               (*File contains numerically searchable property data)
                                                                                           Other Sources: DSL**, EINECS**, TSCA**
                                                                                               (**Enter CHEMLIST File for up-to-date regulatory information)
                                                                                      H3C-C-CH-CH2
                                                                                       **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
                                                                                                  7606 REFERENCES IN FILE CA (1907 TO DATE)
                                                                                                    88 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
                                                                                                  7626 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                                                                                                    77 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
                                                                                                 1: 145:158332
                                                                                      REFERENCE
                                                                                      REFERENCE
                                                                                                 2: 145:156520
                                                                                      REFERENCE
                                                                                                 3: 145:145554
                                                                                      REFERENCE
                                                                                                 4: 145:145400
                                                                                      REFERENCE
                                                                                                  5: 145:145337
                                                                                      REFERENCE
                                                                                                  6: 145:145001
                                                                                      REFERENCE
                                                                                                 7: 145:145000
                                                                                      REFERENCE
                                                                                                 8: 145:144977
                                                                                      REFERENCE 9: 145:131625
L2 ANSWER 96 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
                                                           (Continued)
                                                                                      L2 ANSWER 97 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
                                                                                           78-83-1 REGISTRY
                                                                                           Entered STN: 16 Nov 1984
REFERENCE 10: 145:124765
                                                                                          1-Propanol, 2-methyl- (9CI) (CA INDEX NAME)
                                                                                      OTHER CA INDEX NAMES:
                                                                                      CN Isobutyl alcohol (8CI)
                                                                                      OTHER NAMES:
                                                                                           1-Isobutanol
                                                                                          2-Methyl-1-propanol
                                                                                      CN ·
                                                                                           2-Methylpropyl alcohol
                                                                                           iso-Butyl alcohol
                                                                                      CN
                                                                                           Isobutanol
                                                                                           Isopropyl carbinol
                                                                                      CN
                                                                                           NSC 5708
                                                                                           3D CONCORD
                                                                                      FS
                                                                                           C4 H10 Q
                                                                                      MF
                                                                                      CI
                                                                                           COM
                                                                                      LC
                                                                                           STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO,
                                                                                      CA,
                                                                                             CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST,
                                                                                             CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU, EMBASE, ENCOMPLIT,
                                                                                             ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT,
                                                                                             IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS,
                                                                                             RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2,
                                                                                             USPATFULL, VTB
                                                                                               (*File contains numerically searchable property data)
                                                                                           Other Sources: DSL**, EINECS**, TSCA**
                                                                                               (**Enter CHEMLIST File for up-to-date regulatory information)
                                                                                           CH3
                                                                                      H3C-CH-CH2-OH
                                                                                      **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
                                                                                                 14295 REFERENCES IN FILE CA (1907 TO DATE)
                                                                                                   258 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
                                                                                                 14346 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                                                                                                     6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
                                                                                      REFERENCE 1: 145:158611
                                                                                      REFERENCE
                                                                                                 2: 145:153589
                                                                                      REFERENCE 3: 145:153537
                                                                                      REFERENCE 4: 145:152812
                                                                                      REFERENCE 5: 145:151267
                                                                                      REFERENCE
                                                                                                  6: 145:150394
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REFERENCE

7: 145:148681

REFERENCE 8: 145:148071

L2 ANSWER 97 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued) REFERENCE 9: 145:146195

REFERENCE 10: 145:145808

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Entered STN: 16 Nov 1984
     1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI)
OTHER CA INDEX NAMES:
CN Indole-3-acetic acid, 1-(p-chlorobenzoyl)-5-methoxy-2-methyl- (8CI)
OTHER NAMES:
     a-{1-(p-Chlorobenzoy1)-2-methy1-5-methoxy-3-indoly1)acetic acid
     1-(4-Chlorobenzoyl)-2-methyl-5-methoxyindole-3-acetic acid
    1-(4-Chlorobenzoyl)-5-methoxy-2-methylindole-3-acetic acid
    1-(p-Chlorobenzoyl)-2-methyl-5-methoxy-3-indolylacetic acid
     1-(p-Chlorobenzoyl)-2-methyl-5-methoxyindole-3-acetic acid
     1-(p-Chlorobenzoyl)-5-methoxy-2-methyl-3-indolylacetic acid
     1-(p-Chlorobenzoyl)-5-methoxy-2-methylindole-3-acetic acid
CN
CN
     Amuno
CN
     Argun
CN
     Artracin
CN
    Artrinovo
     Artrivia
ÇN
     Bonidin
ÇN
     Bonidon Gel
     Catlep
CN
     Chibro-Amuno
     Chrono-Indicid
     Chrono-Indocid 75
CN
     Confortid
CN
     Dolcidium
CN
     Dolcidium PL
CN
     Dolovin
CN
     Durametacin
CN
     Elmetacin
CN
     Flam
     Globa
CN
CN
     Idomethine
     Imbrilon
CN
CN
    Inacid
     Indacin
     Indo-Phlogont
CN
     Indo-Rectolmin
     Indo-Tablinen
CN
     Indocid
     Indocid (pharmaceutical)
CN
CN
     Indocin
CN
     Indomecol
     Indomed
CN
CN
     Indomee
CN
     Indometacin
CN
     Indometacine
CN
     Indomethacin
     Indomethacine
CN
     Indomethine
CN
     Indomod
CN
     Indonol
     Indoptic
CN
     Indoptol
     Indorektal
```

ANSWER 98 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN

53-86-1 REGISTRY

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L2 ANSWER 98 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for
     DISPLAY
    3D CONCORD
    503560-73-4, 37242-43-6, 91853-74-6
     C19 H16 C1 N O4
CI
    COM
    STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE,
BEILSTEIN*,
       BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DRUGU, EMBASE, HSDB*,
IFICDB,
       IFIPAT, IFIUDB, IMSCOSEARCH, IMSPATENTS, IPA, MEDLINE, MRCK*, MSDS-OHS,
       PHAR, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE,
       TOXCENTER, ULIDAT, USAN, USPATZ, USPATFULL, VETU
         (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**, WHO
         (**Enter CHEMLIST File for up-to-date regulatory information)
      HO2C-CH2
```

```
** PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
          14519 REFERENCES IN FILE CA (1907 TO DATE)
            205 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
           14534 REFERENCES IN FILE CAPLUS (1907 TO DATE)
             60 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
REFERENCE 1: 145:152718
           2: 145:152695
REFERENCE
REFERENCE 3: 145:152690
REFERENCE
           4: 145:152394
REFERENCE
           5: 145:152347
REFERENCE
           6: 145:152329
REFERENCE
          7: 145:152315
REFERENCE 8: 145:152310
REFERENCE 9: 145:152295
```

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L2 ANSWER 99 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN
     52-67-5 REGISTRY
     Entered STN: 16 Nov 1984
     D-Valine, 3-mercapto- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Valine, 3-mercapto-, D- (BCI)
OTHER NAMES:
     (-)-Penicillamine
ÇN
     (2S)-2-Amino-3-methyl-3-sulfanylbutanoic acid
CN
     (S)-3,3-Dimethylcysteine
CN
     (S)-Penicillamine
CM
     B-Thiovaline
CN
     2-Amino-3-mercapto-3-methylbutanoic acid
     Cuprenil
CN
CN
     Cuprimine
CN
     Cupripen
CN
     D-(-)-Penicillamine
CN
     D-3-Mercaptovaline
     D-Mercaptovaline
     D-Penamine
CN
CN
     D-Penicillamine
CN
     Depamine
     Depen
CN
CN
     DPA
CN
     Kuprenil
CN
     Mercaptyl
CN
     Metalcaptase
     NSC 81549
CN
CN
     Pendramine
CN
     Penicillamin
CN
     Penicillamine
CN
     Perdolat
CN
     Reduced D-penicillamine
CN
     Reduced penicillamine
CN
     Sufirtan
CN
     Trolovol
FS
     STEREOSEARCH
DR
     16414-54-3
MF
     C5 H11 N O2 S
CI
     COM
     STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS,
       BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DRUGU, EMBASE,
       HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS,
NAPRALERT,
       PHAR, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USAN, USPAT2,
       USPATFULL, VETU
         (*File contains numerically searchable property data)
     Other Sources: EINECS**, WHO
         (**Enter CHEMLIST File for up-to-date regulatory information)
Absolute stereochemistry.
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L2 ANSWER 99 OF 99 REGISTRY COPYRIGHT 2006 ACS on STN (Continued)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3296 REFERENCES IN FILE CA (1907 TO DATE)
227 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3300 REFERENCES IN FILE CAPLUS (1907 TO DATE)
24 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 145:152690

REFERENCE 2: 145:139680

REFERENCE 3: 145:137427

REFERENCE 4: 145:136969

REFERENCE 5: 145:122111

REFERENCE 6: 145:119753

REFERENCE 7: 145:96313
REFERENCE 8: 145:95776

REFERENCE 9: 145:95542

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